Potential Intermediates of Aerobic Sulfolane Degradation

Prepared for Loren Garner

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Summary: Sulfolane biodegradation by microorganisms is known to occur readily under aerobic conditions. The intermediates of sulfolane biodegradation under aerobic conditions are unknown, however, some intermediates have been proposed in the literature. In addition, some intermediates resulting from the abiotic transformation of sulfolane under aerobic conditions have also been reported. This brief report shows some *proposed* intermediates that can be assayed for based on previous aerobic biotic and abiotic studies with sulfolane.

Potential Biological Sulfolane Intermediates Under Aerobic Conditions

Sulfolane has been found to be readily biodegradable under aerobic conditions in several laboratory studies (Chou and Swatloski, 1983; Fedorak and Coy, 1996; Greene et al., 1998; Greene et al., 2000; Kim et al., 1999a; Kim et al., 1999b; St. Fort, 2006; Matsui et al., 2009; Lee et al., 2010). While CO₂ and sulfite/sulfate were identified as end products of aerobic microbial sulfolane biodegradation (Greene et al., 2000), no other intermediates have yet been identified. However, based on analogy with intermediates known to be formed during the biodegradation of dibenzothiophene sulfone, Greene et al. (2000) predicted that 4-hydroxy-butanesulfinic acid and butanol are also potential intermediates under aerobic conditions (Figure 1). In this proposed aerobic pathway, sulfolane is activated by a monooxygenase to produce 4-hydroxy-butanesulfinic acid, which can then be acted upon by a desulfinase, forming 1-butanol. In this pathway, sulfite would be released and oxidized to sulfate (experimentally observed by Greene et al., 2000), while 1-butanol would presumably be bioconverted to butyraldehyde then butanoic acid (common microbial pathway for bioconversion of an alcohol to a carboxylic acid) that would readily enter into central metabolic pathways leading to CO₂ production.

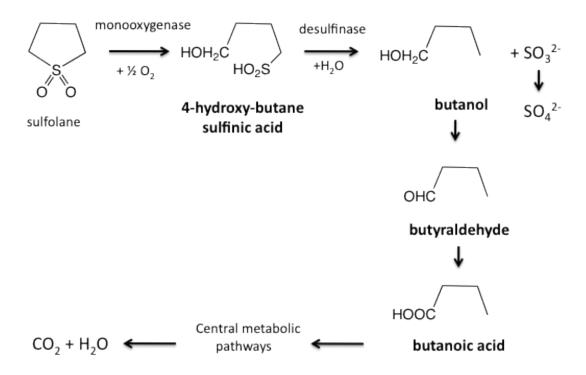


Figure 1. Potential intermediates (shown in bold text) of sulfolane biodegradation under aerobic conditions. Modified from Greene et al., 2000.

Potential Abiotic Sulfolane Intermediates Under Aerobic Conditions

A study conducted by Wellisch et al. (1964) showed that sulfolane can be subject to abiotic transformation under aerobic conditions in the presence of metals such as sodium. Figure 2 shows that under such conditions, sulfolane can be converted to butanesulfinate and octane-1,8-disulfinate (intermediates 1 and 2 in the boxed area) (after Wellisch et al., 1964).

Potential Aerobic Biodegradation Intermediates from Abiotic Sulfolane Intermediates Under Aerobic Conditions

If generated, the abiotic intermediates shown in Figure 2 can then potentially be biodegraded under aerobic conditions to other intermediates. For example, Greene et al. (2000) proposed that monooxygenases and desulfinases could be important enzymes involved in the biological degradation of sulfolane (see Figure 1). These enzymes may also play a role in the biodegradation of any potentially generated abiotic sulfolane intermediates. For example, butanesulfinate (abiotic intermediate 1, Figure 2) could potentially be acted on by a monooxygenase to produce 4-hydroxy-butanesulfinate (intermediate 3), which could in turn be converted by a desulfinase to butanol (intermediate 4). In a similar manner, the abiotically-produced octane-1,8-disulfinate could be biologically transformed by a desulfinase to octane-1-sulfinate (intermediate 5) which in turn may be acted on by a monooxygenase yielding 8-hydroxy-octanesulfinate (intermediate 6). Finally, another desulfinase reaction could yield octanol (intermediate 7) (Figure 2). Butanol and octanol would then be rapidly biodegraded through the corresponding aldehyde and carboxylic acid that would then enter central metabolic pathways leading to CO₂ production.

It must be reiterated that the potential biological intermediates shown in Figures 1 and 2 are hypothetical, and have not been found in any aerobic sulfolane biodegradation studies conducted to date.

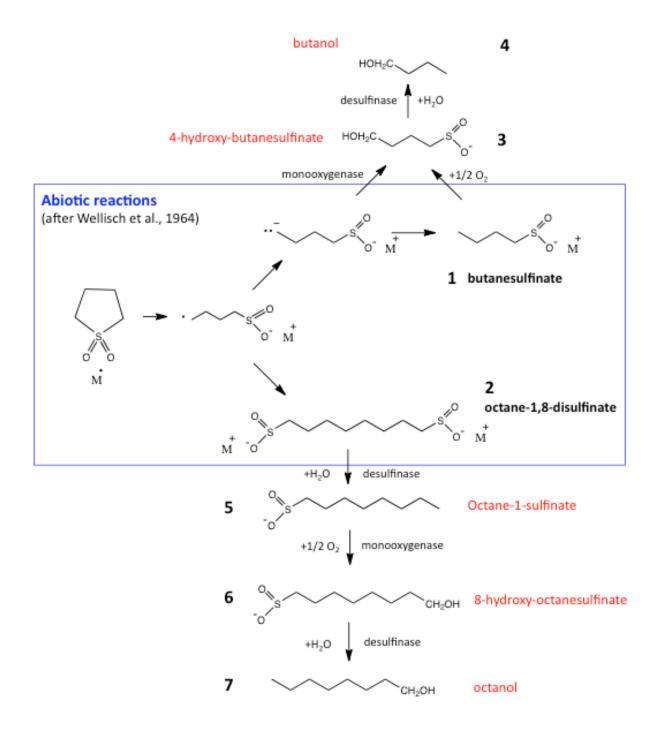


Figure 2. Potential intermediates of sulfolane abiotic degradation and subsequent biotic degradation under aerobic conditions. Abiotic reactions/products are shown in the boxed area (intermediates 1 & 2, after Wellisch et al., 1964). Other potential intermediates (3 – 7) are proposed aerobic biological intermediates that may result from the subsequent biodegradation of the abiotic products.

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